Propylbenzene 103-65-1 | DTXSID3042219

Model Performance

Model	Data

Weighted KNN model

5-fold CV (5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 160 °C

Global applicability domain: Inside

Local applicability domain index: 7.86e-01

Confidence level: 9.04e-01

Nearest Neighbors from the Training Set

Image not found
Propylbenzene

Measured: 159 Predicted: 160 Image not found

3-Ethyltoluene Measured: 161 Predicted: 160 Image not found

1-Ethyl-2-methylbenzene

Measured: 165 Predicted: 160

Image not found

4-Ethyltoluene Measured: 162 Predicted: 160 Image not found

Cumene Measured: 152 Predicted: 160